Watermatex 2019

Plant-wide optimization through dynamic compartmental modelling and analysis of limiting processes.

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Abstract: The current Tanks in Series (TIS) approach used to model the hydrodynamics of Water and Resource Recovery Facilities lacks in spatial detail to address most modelling goals, including reactor design and predictions during wet weather. On the other hand, advanced CFD simulations to reach these goals are often too time-consuming. This paper investigates an intermediate model structure, named Compartmental Model (CM), in terms of prediction capacity compared to the classic TIS approach. It does so in the context of a plant-wide model, by comparing online data with simulations from a TIS model and two types of CMs, static and dynamic. Results show that this new model structure indeed improves the prediction quality on several fronts. Further improvements, both in model performance and compartimentalisation methodology, are still challenging.

Keywords: Compartmental Modeling; plant-wide modeling; process limitations

Introduction

Hydrodynamic modelling of Water & Resource Recovery Facilities (WRRFs) is, at least within flow-sheet tools, currently mostly based on a Tanks-In-Series (TIS) approach. This approach conceptually divides a bioreactor into multiple completely mixed tanks in only one dimension, i.e. the direction of the bulk flow. Variations in the other two dimensions are not taken into account, although these do occur in reality, causing for example mass transfer-limited zones or short circuiting. This makes the TIS approach oversimplified; it does not contain the hydrodynamic detail needed to achieve several common modelling goals such as reactor design evaluation, the development of precise control strategies or model development for both dry and wet weather, i.e. without the need for recalibration.

A solution to this problem can come in the form of Computational Fluid Dynamics (CFD) simulations, modelling hydrodynamics in a very detailed way, even including biokinetics. However, the use of CFD as a mainstream WRRF modelling tool is limited, mainly due to its high computational demands and the increased need for detailed validation data. An intermediate modelling approach with sufficient hydrodynamic detail and manageable calculation times seems appropriate. Such an intermediate model structure, named a Compartmental Model (CM), has been the topic of previous research already (Alex et al., 2002; Rehman, 2016). Rehman (2016) developed a method that uses a detailed CFD(-biokinetic) model to construct a Compartmental Model that describes a reactor as a conceptual network of spatially localized compartments, connected through convective and exchange fluxes. Relatively new in the context of WRRF modelling, this Compartmental Model structure has only been applied in a very limited number of cases, made use of fixed compartment volumes and fluxes and has never been validated on a full scale WRRF (Gresch et al., 2009; Le Moullec et al., 2011). This paper deepens the knowledge on CMs by applying the model structure to an available plant-wide model and by making the compartment volumes dynamically dependent on factors well-known for affecting the hydrodynamic patterns (e.g. influent flow rate and air flow rate to the considered tank) using a surrogate model. Both CM and TIS simulations are compared to full-scale data.

Material and Methods

As case study, the WRRF of Eindhoven (The Netherlands) operated by Waterboard De Dommel is taken. The main treatment processes used at the Eindhoven WWTP include primary settling, activated sludge treatment and secondary clarification. The activated sludge treatment features a modified UCT layout (Figure 1A), in order to enhance the biological phosphorous removal at the plant. This layout consists of an anaerobic inner ring (with a volume of 11,196 m³), an anoxic middle ring (with a volume of 28,750 m³) and an aerobic-anoxic outer ring (with a volume of 50,311 m³). The aerobic-anoxic outer ring contains two zones where aeration is possible, the so-called summer and winter aeration packages. In this study the main focus is the outer ring as it is believed that the aeration, in combination with the sheer size and the concentric design, results in a complex hydraulic pattern for which an TIS approach is deemed to be an oversimplification of reality.

Figure 1 gives a schematic layout of both the TIS model (Figure 1C) and the CM (Figure 1D), as well as an intermediate figure (Figure 1B) clarifying the construction of the CM. Only the outer, aerated ring of the Eindhoven WRRF is provided with a CM layout, because, as stated above, the TIS assumptions are least likely to be valid there. This CM is then included in the available plant-wide model.

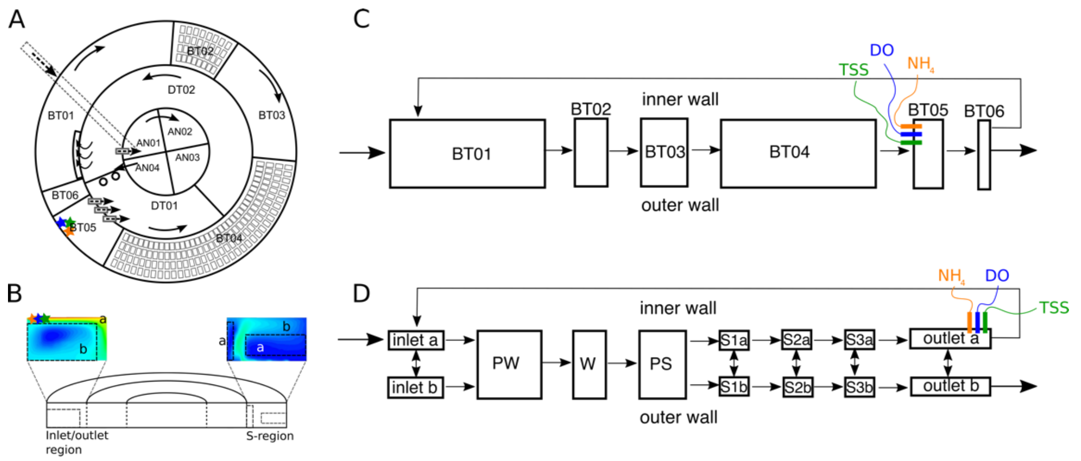

Figure 1.(A) Configuration, (B) CFD-biokinetic model slices, (C) TIS model & (D) Compartmental Model of the Eindhoven WRRF outer ring. Blue, orange and green elements indicate the location of dissolved oxygen, ammonium and Total Suspended Solids probes resp. AN: anaerobic inner ring, DT: anoxic middle ring, BT: aerobic outer ring, PW: Pre-Winter aeration package, W: Winter aeration package, PS: Pre-Summer aeration package, S: Summer aeration packages.

Important to notice is the implementation of the aeration. Whereas in the TIS model aeration happened in two out of six tanks (BT02 and BT04, representing resp. the winter and summer aeration package), this is the case for four compartments out of thirteen in the CM. The implementation of the aeration of BT02 (corresponding to the WINTER compartment in the CM) stays unchanged, but the airflow rate to the summer aeration package as calculated by the controller in the plant-wide model now needs to be distributed over resp. S1a, S2a and S3a (Figure 1D), instead of just sent to BT04.

Because these three volumes are equal within the CM, this distribution can also happen equally: the airflow rate can be divided by three and sent to the relevant compartments. The choice of sending air only to the a-compartments and not to the b-compartments is based on the CFD simulation results, that predict the a-compartments to have much higher dissolved oxygen concentrations. This assumes that the only way oxygen can enter the b-compartments is by means of advection of already dissolved oxygen into those zones. Further experiences will have to show whether this assumption holds or not.

Also the location of both the ammonium and Dissolved Oxygen (DO) sensors is important. Based on the actual location at the plant, the corresponding location in the CM is in compartment outlet a.

Next to aeration, specific attention has been given to the location of the recycles and the mapping of the location on the CM. It is for example not possible for water to go from the outside of the outer ring (b-compartments) to the nitrate recycle flow, which can only come from a-compartments. Likewise, the effluent can in theory only come from the b-compartments.

Simulating dynamically (i.e. with varying influent flow rates and/or loads) with the plant-wide model including the CM is already possible at this point, but will possibly loose predictive capacity as soon as the dynamics bring the simulation too far from the steady state situation the CM is based on. To mitigate this, a CM is developed in which the compartment volumes and the exchange flow rates between the compartments are dynamically calculated by a surrogate model during the simulation.

A surrogate model is a compact, approximate model constructed based on the output of a complex, computational expensive model (Gorissen et al. 2010), here the CFD model. Because dynamic CFD and especially CFD-ASM simulations are to date not yet possible with reasonable simulation times (in the order of minutes), these dynamic volumes and exchange flows are approximated based on several steady state situations combined with assumptions about the transition between them.

For the case study at hand, the results of 14 available CFD-scenarios were analysed in order to make the CM dynamic. Compartment volumes for each scenario were determined based on the methodology of Rehman (2016). A linear-parabolic function was then fitted to these volumes, where the description of each (relative) compartment volume as function of influent flow rate was linear and that same (relative) volume as function of the air flow rate was parabolic. The fitting made use of weights based on the frequency of occurrence of each scenario. This yielded a so-called surrogate model for each volume in function of the influent flow rate and the air flow rate entering the outer ring (see Figure 1A) of the plant.

To support the development of the compartmental models, the colour analysis tool developed in Amerlinck et al. (2015) was used. This allowed to determine whether model outputs could be attributed to substrate limitations, or directly to the changes in hydrodynamic model structure.

Comparison of the three model structures (TIS, fixed CM and dynamic CM) happened on a visual basis, by comparing model predictions with available on-line data obtained at the plant between November 16 and December 8, 2013.

Results and Discussion

For the total suspended solids (TSS) concentration in the biological tanks, all three models give very comparable predictions. Differences are more pronounced in the model predictions for dissolved oxygen (DO), ammonium (NH_4) and nitrate (NO_3) concentrations.

Figure 2 shows the comparison between the model predictions with data for DO and air flow rates. In addition, Figure 3 shows the comparison for the nitrogen species, i.e. ammonium (NH_4) concentrations in the outer ring and nitrate (NO_3) concentrations in both the middle and inner ring. Dissolved oxygen concentration in the last part of the aerobic outer ring (compartments BT06 and outlet a for resp. the TIS and the CM models) is predicted reasonably to very well by all three models (Figure 2 top). Differences mostly concern the actual values of the predictions, while in terms of dynamics, all three models are comparable and prediction dynamics are similar to those in the measurements. The tendency of the TIS model to underestimate the DO level is explained as follows. The TIS model assumes the last part of the aerobic tank (BT06) to be completely mixed in the direction perpendicular to the flow, while the hydrodynamic reality is that this part is better represented by two zones, like applied in the CMs. The TIS predictions therefore effectively average out the concentration in the last part of the outer ring, and end up at a lower value than that of the actual measurement, which is measured in the oxygen-rich zone.

The airflow rate over the entire summer package (Figure 2 bottom) is often overestimated by the TIS model. In fact, this overestimation is to a lesser extent also present in the CM predictions, although in those cases, the complete range of values better matches that of the data. Just like for the DO concentrations, dynamics in the models are very comparable and correspond with the data to a large extent.

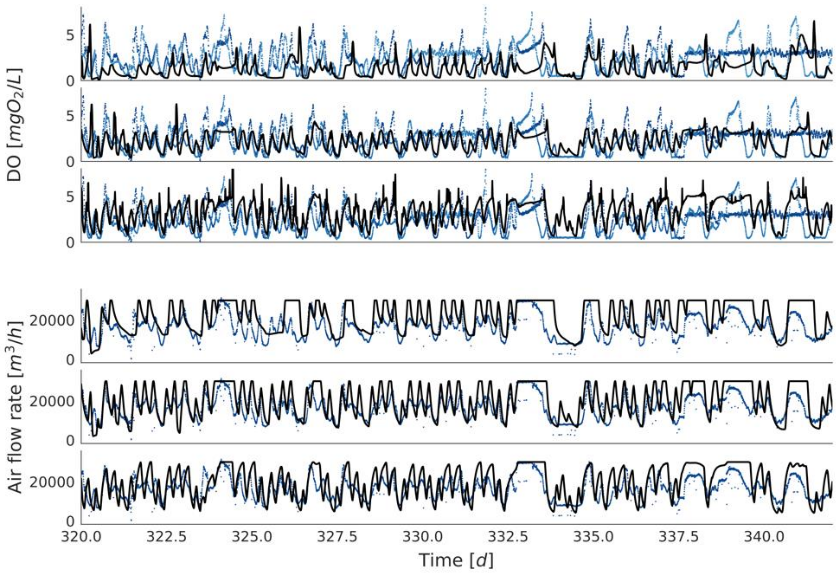

Figure 2. Top three graphs: Dissolved oxygen concentration in the last part of the outer ring (OUT_A for the CMs). Bottom three graphs: total air flow rate entering the outer ring. Both in the top and bottom graph, from top to bottom: TIS, Fixed CM, Dynamic CM. Lines: predictions; dots: data.

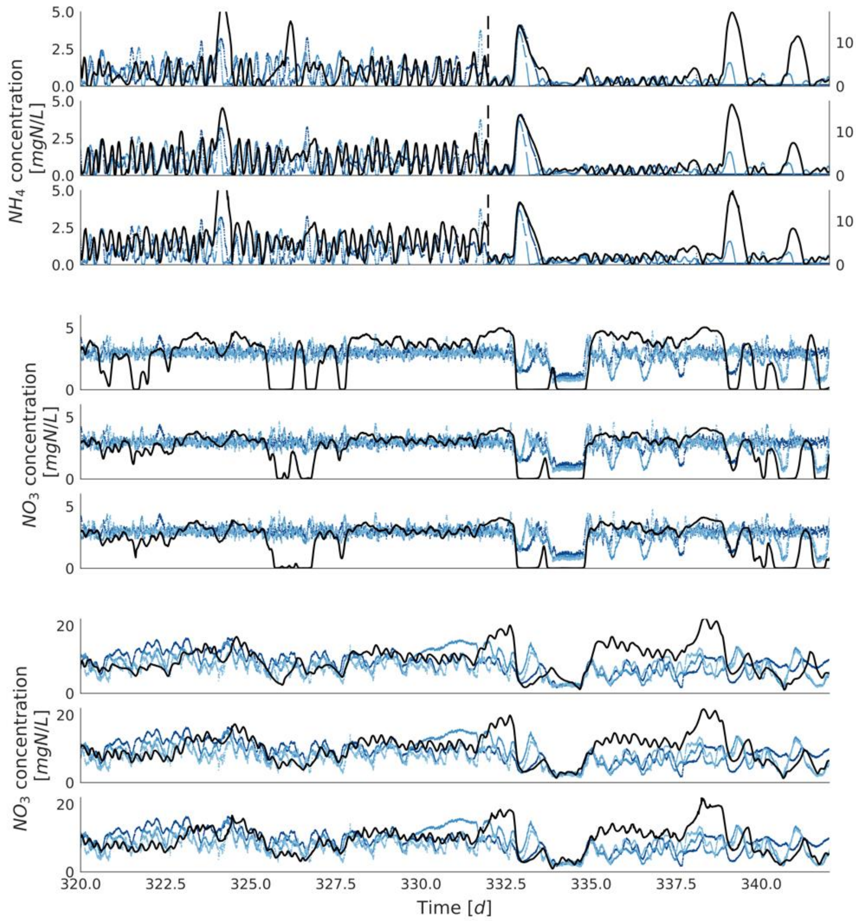

Figure 3. Top three graphs: Ammonium concentration in the last part of the outer ring. Middle three graphs: Nitrate concentration in the middle ring. Bottom three graphs: Nitrate concentration in the outer ring. For all three graphs (Top, middle and bottom), from top to bottom: TIS, Fixed CM, Dynamic CM. Lines: predictions; dots: data.

The best predictions for the ammonium concentration near the end of the aerobic outer ring are done by the CM with fixed volumes and exchange flows (Figure 3 top): especially in dry weather (left of the dashed line), both dynamics and range of the measured values are matched accurately. The overestimations made by all three models under wet weather conditions (right of the dashed line) were found hard to explain purely based on the (combined) validation graphs; clearly there is a difference in effect between the first rain event, which is indeed represented correctly in terms of ammonium concentration, and the two following ones.

With regards to nitrate concentrations in the middle ring (Figure 3 middle), it is clear that both CMs again yield better predictions than the TIS model. Between the CMs, differences are minimal. Nitrate predictions at the end of the outer ring (Figure 3 bottom) are similar in quality between all three model structures: reasonable, but (on a visual basis at least) not as accurate as the prediction of most other variables. Note that also the nitrate measurements themselves seem to be less similar in between the three parallel lanes than other variables.

The reason for peak overestimation of ammonium in all three models can be either a limitation in autotrophic biomass, substrate limitation, or badly represented hydrodynamics (and so residence times). To estimate the impact of substrate limitations on nitrification, the color-based model analysis methodology of Amerlinck et al. (2015)

was applied. Figure 4 reveals that the most severe substrate limitations to the nitrification rate surprisingly do not occur during (the first two) rain events, while ammonium concentrations do peak under those conditions. Further investigation showed that it is indeed a decreased residence time of autotrophs leading to the overestimations in ammonium concentration (results not shown). Despite the improved representation of hydrodynamics, the updated model structure still seems to miss important elements, either still situated in a hydrodynamics context, or in the settling process modelling.

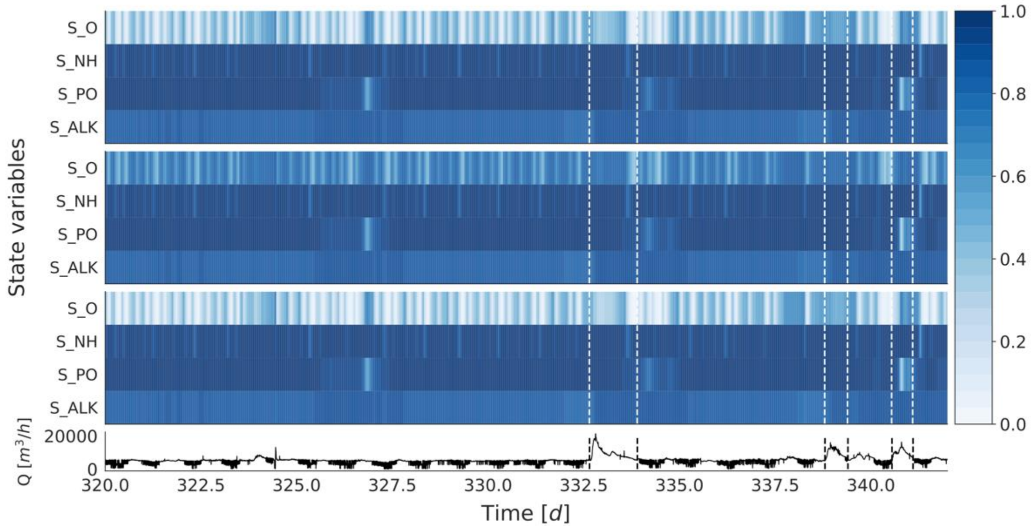

Figure 4. Results of the color-based model analysis developed by Amerlinck et al. (2015) applied to the SUMMER 1 compartments of the dynamic CM of the Eindhoven WWTP. The calculated limitations are based on concentrations of the flow entering the SUMMER 1 compartments (first graph), concentrations in the S1a-compartment (second graph) and concentrations in the S1b-compartment (third graph). A value of 0 means severe limitation, a value of 1 indicates no limitation. Bottom: influent flow to the plant; dashed vertical lines indicate rain events.

Conclusions

In conclusion, both compartmental model structures provide predictions of equal or better quality than the TIS model structure, strongly indicating that modeling with increased hydrodynamic detail (1) is already valuable, (2) is attainable with simulation times similar to those of TIS models and (3) still has a large potential to improve. The added value of a dynamic compartmental model could not be distinguished based on current results. The combination of the shown potential of compartmental models and the current limitations of the dynamic compartmental model do justify further research in that direction, even if only to establish the presence or absence of the added value of dynamic compartmental models.

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